Polynomial Neural Sheaf Diffusion: A Spectral Filtering Approach on Cellular Sheaves

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Introduction & Background

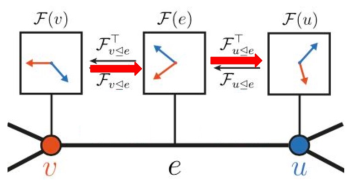
❌ **PROBLEM**

Most of GNNs present an accuracy degradation in heterophilic settings/when adding many layers:

- Rely on the **Homophilic Assumption**.
- Suffer from **Oversmoothing Effect**.

✅ **SOLUTION → SHEAF NEURAL NETWORKS**

- **False Assumption**: Graph Nodes live in the same global feature space.
- Assign a vector space (**stalk**) to each node and edge and learn **restriction maps** (and transport maps) among them.



How to move a vector x from v to u?

Moving $\mathbf{x} \in \mathcal{F}(v) \to \mathcal{F}(u)$ is done via maps composition!

$$\mathcal{F}^{\top}_{u\trianglelefteq e}\mathcal{F}_{v\trianglelefteq e}\,\mathbf{x} \in \mathcal{F}(u)$$

Sheaf Laplacian

Q: Can we measure the **total disagreement** at each node?

- Space of 0-Cochains: $C^0(\mathcal{G},\mathcal{F}) := \bigoplus_{u\in\mathcal{V}} \mathcal{F}(u)$
- Space of 1-Cochains: $C^1(\mathcal{G},\mathcal{F}) := \bigoplus_{e\in\mathcal{E}} \mathcal{F}(e)$
- Co-boundary Map: $\delta : C^0(\mathcal{G},\mathcal{F}) \to C^1(\mathcal{G},\mathcal{F})$
  - ↳ Measures the nodes disagreement

A: Build the **Sheaf Laplacian** $L_{\mathcal{F}} := \delta^{\top}\delta$

$$L_{\mathcal{F}}(\mathbf{x})_u = \sum_{u,v\trianglelefteq e} \mathcal{F}^{\top}_{u\trianglelefteq e}(\mathcal{F}_{u\trianglelefteq e}\mathbf{x}_u - \mathcal{F}_{v\trianglelefteq e}\mathbf{x}_v)$$

Polynomial Neural Sheaf Diffusion

- Model-agnostic SheafNN framework to perform diffusion explicitly in the spectral domain.
- Applies Orthogonal Polynomials filters to the spectrally rescaled sheaf Laplacian.
- No need anymore for large stalk dimensions.
- Same asymptotic cost of stacking K NSD-layers but without Laplacian re-assembly.

Double Interpretation:

1. **Spectral**: Frequency–selective filter on the sheaf signal.
2. **Spatial**: The degree K determines the receptive field, mixing information across all paths of length up to K in a single pass.

$$p(\lambda) = \sum_{k=0}^{K} \theta_k B_k(\,\tilde{L}\,), \qquad \tilde{L} = \frac{2}{\lambda_{\max}} L - I$$

Research Question

Current SNNs still rely on 1^{st} order spatial diffusion: reaching distant nodes requires layer depth, parameter-heavy stalks and dense per-edge maps. Can we solve this?

Long-Range Influence

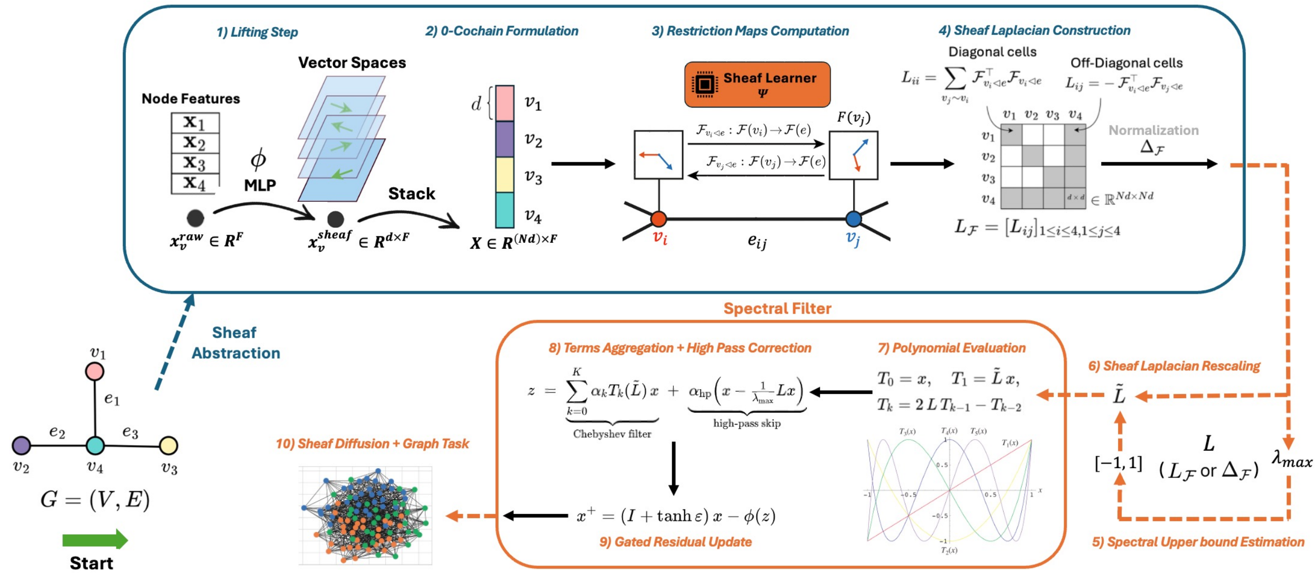
⚠️ Long-range interactions require stacking many layers.
→ Increase computational cost and intensifying the oversmoothing.

🤩 Explicit K-hop receptive field/diffusion/long-range mixing within a single layer.

🥷 Controllable frequency-selective operator, enabling direct control over the diffusion behaviour (low-, band-, or high-pass).

→ Gradient-based Influence Decay to demonstrate persistent Long-Range influence.

$$I(d) := \mathbb{E}_{v\in\mathcal{T}}\left[\frac{1}{|\mathcal{N}_d(v)|}\sum_{u\in\mathcal{N}_d(v)} G_{uv}\right]$$



Experiments & Results

Discrete Models

	Texas	Wisconsin	Film	Squirrel	Chameleon	Cornell	Citeseer	Pubmed	Cora
Homophily	**0.11**	**0.21**	**0.22**	**0.22**	**0.23**	**0.30**	**0.74**	**0.80**	**0.81**
#Nodes	183	251	7,600	5,201	2,277	183	3,327	18,717	2,708
#Edges	295	466	26,752	198,493	31,421	280	4,676	44,327	5,278
#Classes	5	5	5	5	5	5	7	3	6
DiagPolySD	90.00±4.68	88.63±3.59	37.31±0.98	56.61±2.06	71.45±2.03	86.49±5.54	77.74±1.26	89.70±0.32	88.79±1.13
BundlePolySD	89.74±5.32	89.41±4.04	37.47±0.86	55.76±2.02	71.18±1.46	86.76±4.90	77.57±1.55	89.75±0.34	88.33±1.34
GeneralPolySD	89.21±5.05	88.82±4.89	37.34±1.13	55.79±2.52	69.62±1.85	86.49±5.80	77.21±1.58	89.73±0.41	88.47±1.19
PolySpectralGNN	64.59±6.40	58.62±6.04	25.50±0.85	51.72±1.76	62.65±3.03	54.59±6.26	60.40±0.89	78.70±0.56	76.20±0.67
ChebNetII	68.42±6.96	64.76±6.93	32.39±4.45	47.06±1.74	63.23±5.83	80.40±5.56	72.00±1.66	85.87±3.34	85.35±6.75
BernNet	73.68±6.00	63.65±6.76	30.23±6.34	46.47±1.47	61.00±2.34	76.87±5.26	65.29±5.55	83.94±3.83	84.76±4.75
RiSNN	86.84±3.72	87.84±2.60	*N/A*	53.30±3.30	65.15±2.40	85.95±6.14	76.23±1.81	88.00±0.42	85.27±1.11
JdSNN	87.37±5.10	89.22±3.42	*N/A*	49.89±1.71	66.40±2.33	85.41±4.55	73.27±1.86	88.19±0.55	85.43±1.73
Conn-NSD	86.16±2.24	88.73±4.47	37.91±1.28	45.19±1.57	65.21±2.04	85.95±7.72	75.61±1.93	89.28±0.38	83.74±2.19
Diag-NSD	85.67±6.95	88.63±2.75	37.79±1.01	54.78±1.81	68.68±1.73	86.49±7.35	77.14±1.85	89.42±0.43	87.14±1.06
O(d)-NSD	85.95±5.51	89.41±4.74	37.81±1.15	56.34±1.32	68.04±1.58	84.86±4.71	76.70±1.57	89.49±0.40	86.90±1.13
Gen-NSD	82.97±5.13	89.21±3.84	37.80±1.22	53.17±1.31	67.93±1.58	85.68±6.51	76.32±1.65	89.33±0.35	87.30±1.15
GGCN	84.86±4.55	86.86±3.29	37.54±1.56	55.17±1.58	71.14±1.84	85.68±6.63	77.14±1.45	89.15±0.37	87.95±1.05
H2GCN	84.86±7.23	87.65±4.98	35.70±1.00	36.48±1.86	60.11±2.15	82.70±5.28	77.11±1.57	89.49±0.38	87.87±1.20
GCNII	77.57±3.83	80.39±3.40	37.44±1.30	38.47±1.58	63.86±3.04	77.86±3.79	77.33±1.48	90.15±0.43	88.37±1.25
GraphSAGE	82.43±6.14	81.18±5.56	34.23±0.99	41.61±0.74	58.73±1.68	75.95±5.01	76.04±1.30	88.45±0.50	86.90±1.04
GCN	55.14±5.16	51.76±3.06	27.32±1.10	53.43±2.01	64.82±2.24	60.54±5.30	76.50±1.36	88.42±0.50	86.98±1.27
GAT	52.16±6.63	49.41±4.09	27.44±0.89	40.72±1.55	60.26±2.50	61.89±5.05	76.55±1.23	87.30±1.10	86.33±0.48
MLP	80.81±4.75	85.29±3.31	36.53±0.70	28.77±1.56	46.21±2.99	81.89±6.40	74.02±1.90	75.69±2.00	87.16±0.37

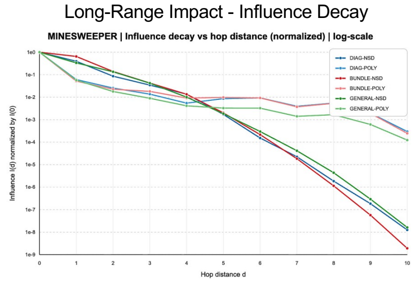
Method	Cham.-Filt.	Squi.-Filt.	Roman	Amazon	Mine.	Tolok.	Quest.
ResNet	36.73 ± 4.71	36.55 ± 1.82	65.88 ± 0.38	45.90 ± 0.52	50.89 ± 1.39	72.95 ± 1.06	70.34 ± 0.76
GCN	40.89 ± 4.12	39.47 ± 1.47	73.69 ± 0.74	48.70 ± 0.63	89.75 ± 0.52	83.64 ± 0.67	76.09 ± 1.27
SAGE	37.77 ± 4.14	36.09 ± 1.99	85.74 ± 0.67	53.63 ± 0.39	93.51 ± 0.57	82.43 ± 0.44	76.44 ± 0.62
GT-sep	40.31 ± 3.01	36.66 ± 1.63	87.32 ± 0.39	52.18 ± 0.80	92.29 ± 0.47	82.52 ± 0.92	78.05 ± 0.93
FAGCN	41.90 ± 2.72	41.08 ± 2.27	65.22 ± 0.56	44.12 ± 0.30	88.17 ± 0.73	77.75 ± 1.05	77.24 ± 1.26
FSGNN	40.61 ± 2.97	35.92 ± 1.32	79.92 ± 0.56	52.74 ± 0.83	90.08 ± 0.70	82.76 ± 0.61	78.86 ± 0.92
ChebNetII	40.82 ± 4.96	41.09 ± 2.41	63.86 ± 0.43	38.82 ± 0.07	74.73 ± 1.51	75.09 ± 0.87	68.50 ± 1.55
BernNet	37.30 ± 4.17	42.41 ± 1.97	67.46 ± 4.38	36.79 ± 0.05	80.94 ± 1.16	76.19 ± 0.85	66.35 ± 1.23
PolySpectralGNN	38.25 ± 5.33	41.24 ± 1.87	59.16 ± 1.64	36.98 ± 0.64	86.59 ± 0.60	78.20 ± 0.61	69.40 ± 1.74
NSD-Diag	41.05 ± 4.01	43.11 ± 2.09	76.82 ± 2.49	38.79 ± 0.39	86.34 ± 0.69	75.31 ± 1.14	69.94 ± 2.04
NSD-Bundle	40.56 ± 2.67	42.43 ± 3.23	78.75 ± 2.23	40.23 ± 0.23	87.43 ± 0.96	78.65 ± 2.94	66.23 ± 1.49
NSD-General	42.72 ± 2.06	43.71 ± 2.06	80.41 ± 0.72	42.76 ± 0.54	92.15 ± 0.84	80.31 ± 0.76	69.69 ± 1.46
PolyNSD-Diag	45.88 ± 3.60	48.60 ± 1.85	87.49 ± 2.21	52.87 ± 0.24	96.98 ± 0.55	82.27 ± 0.61	75.37 ± 1.08
PolyNSD-Bundle	44.64 ± 3.78	47.86 ± 1.79	88.54 ± 1.65	53.87 ± 0.28	97.23 ± 0.55	83.92 ± 0.61	76.37 ± 1.08
PolyNSD-General	45.94 ± 3.79	48.82 ± 1.60	89.87 ± 1.36	54.34 ± 0.34	98.86 ± 0.55	84.75 ± 0.61	79.37 ± 1.08

- ▶ New s.o.t.a. results on heterophilic and homophilic datasets.
- ▶ Diag models invert NSD* trend → performances speed-up.
- ▶ Stalk dimension has not big impact as it was for NSD.
- ▶ No Oversmoothing →High results if L increases.
- ▶ Same is valid for the Continuous Neural Sheaf Diffusion.

Continuous Models

	Texas	Wisconsin	Film	Squirrel	Chameleon	Cornell	Citeseer	PubMed	Cora
Homophily	**0.11**	**0.21**	**0.22**	**0.22**	**0.23**	**0.30**	**0.74**	**0.80**	**0.81**
#Nodes	183	251	7,600	5,201	2,277	183	3,327	18,717	2,708
#Edges	295	466	26,752	198,493	31,421	280	4,676	44,327	5,278
#Classes	5	5	5	5	5	5	7	3	6
Cont DiagChebySD	86.58±5.45	88.04±3.45	36.80±1.01	53.76±1.78	65.74±3.50	84.86±5.30	76.71±1.63	89.58±0.46	87.83±1.19
Cont BundleChebySD	86.84±7.16	86.47±6.17	37.42±1.12	52.34±2.43	66.49±1.55	84.59±5.27	75.66±1.60	89.70±0.31	87.73±1.26
Cont GeneralChebySD	83.42±5.53	86.86±3.40	36.76±0.96	52.87±1.89	64.10±2.35	84.86±4.22	76.01±2.03	89.32±0.38	87.79±1.34
Cont Diag-NSD	82.97±4.37	86.47±2.55	36.85±1.21	38.17±9.29	62.06±3.84	80.06±6.07	76.56±1.19	89.47±0.42	86.88±1.21
Cont O(d)-NSD	82.43±5.95	84.50±4.34	36.39±1.37	40.40±2.01	63.18±1.69	72.16±10.40	75.19±1.67	89.12±0.30	86.70±1.24
Cont Gen-NSD	83.78±6.62	85.29±3.31	37.28±0.74	52.57±2.82	66.40±2.28	84.60±4.68	77.54±1.72	89.67±0.40	87.45±0.99
BLEND	83.24±4.65	84.12±3.58	35.63±0.89	43.06±1.39	60.11±2.09	85.95±6.82	76.63±1.60	89.24±0.42	88.09±1.22
GRAND	75.68±7.25	79.41±3.64	35.62±1.01	40.05±1.50	54.67±2.54	82.16±7.09	76.46±1.77	89.02±0.52	87.36±0.96
CGNN	71.35±4.05	74.31±7.26	35.95±0.86	29.24±1.09	46.89±1.69	66.22±7.62	76.91±1.81	87.70±0.49	87.10±1.35

Long-Range Impact - Influence Decay



PolyNSD VS NSD – #Layers Ablation

Layers	**2**	**4**	**8**	**16**	**32**	**Best**	**PolySD Improvement**
PubMed (h=0.80, $\#N = 18{,}707$, $\#E = 44{,}327$, $\#C = 3$) — **DiagChebySD**: 88.18±0.40 (K=8), #params=48,665; **BundleChebySD**: 87.91±0.32 (K=4), #params=49,621; **GeneralChebySD**: 87.87±0.49 (K=8), #params=52,505							
Diag-NSD	87.82±0.55	87.92±0.51	87.92±0.52	65.92±20.39	39.49±1.60	4	+0.26%
#params	48,655	50,507	54,211	61,619	76,435	50,507	-3,65% (-1,842)
Bundle-NSD	87.70±0.56	87.85±0.42	87.94±0.36	87.63±0.47	37.03±4.72	8	-0.03%
#params	49,615	52,427	58,051	69,299	91,795	58,051	-14,52% (-8,430)
General-NSD	87.48±0.64	87.62±0.36	87.72±0.68	39.94±1.03	39.33±2.25	8	+0.15%
#params	52,495	58,187	69,571	92,339	137,875	69,571	-24,53% (-17,066)
Chameleon (h=0.23, $\#N = 2{,}277$, $\#E = 31{,}421$, $\#C = 5$) — **DiagChebySD**: 70.57±1.32 (K=16), #params=194,835; **BundleChebySD**: 66.64±2.35 (K=8), #params=195,787; **GeneralChebySD**: 67.39±2.50 (K=16), #params=198,675							
Diag-NSD	64.43±2.06	61.27±5.14	57.34±6.10	22.92±1.42	22.89±2.59	2	+6.15%
#params	194,817	196,669	200,373	207,781	222,597	194,817	+0.009% (+18)
Bundle-NSD	47.10±10.14	54.08±6.30	50.57±3.53	24.91±2.87	23.05±2.46	4	+12.56%
#params	195,777	198,589	204,213	215,461	237,957	198,589	-1,41% (-2,802)
General-NSD	59.60±4.53	58.18±3.56	26.05±3.41	23.79±3.41	20.07±3.74	2	+7.79%
#params	198,657	204,349	215,733	238,501	284,037	198,657	+0% (+0)
Squirrel (h=0.22, $\#N = 5{,}201$, $\#E = 198{,}493$, $\#C = 5$) — **DiagChebySD**: 47.72±1.20 (K=16), #params=174,675; **BundleChebySD**: 44.48±3.22 (K=16), #params=176,913; **GeneralChebySD**: 42.02±2.50 (K=6), #params=179,785							
Diag-NSD	41.98±1.17	42.60±1.83	42.05±1.54	20.80±1.33	OOM	4	+5.12%
#params	175,937	177,789	181,493	188,901	N/A	177,789	-1,75% (-3,114)
Bundle-NSD	42.46±1.45	42.30±1.83	37.99±2.61	22.86±3.03	OOM	2	+2.02%
#params	176,897	179,709	185,333	196,581	N/A	176,897	+0.009% (+16)
General-NSD	39.11±1.96	39.96±1.76	33.69±1.32	OOM	OOM	4	+2.06%
#params	179,777	185,469	196,853	N/A	N/A	185,469	-3.06% (-5,684)

- ▶ Pick best K for the three models and run #layers and #channels ablation.
- ▶ PolyNSD has low K for homophilic and high K for heterophilic datasets.
- ▶ Even if more layers/hidden channels, PolyNSD is better → Parameter Savings.

*C. Bodnar, F. Di Giovanni, B. Chamberlain, P. Lio, and M. Bronstein. Neural Sheaf Diffusion: A topological perspective on heterophily and oversmoothing in GNNs. *NeurIPS*, 2022.